Modeling of semiconductor defect properties to extend experimental characterization capabilities

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Abstract

Semiconductors are intentionally or unintentionally exposed to radiation of energetic particles during processing (ion implantation for doping or ion beam nanopatterning) or during operation (radiation detectors or devices exposed to cosmic radiation). In any case, as energetic particles enter into a crystalline solid and collide with lattice atoms, defects are generated. The interaction and accumulation of structural defects in crystalline semiconductors can lead to phase transformation (crystalline to amorphous [1]), nanostructure formation (honeycombs in germanium [2]) or dopant deactivation (via clustering or precipitation [3]). Structural defects also lead to shallow or deep levels in the gap and may also act as additional scattering centers. This often has adverse effects on the performance of logic devices (increase of leakage currents), the efficiency of solar cells (reduce the charge collection efficiency) or lifetime of radiation detectors (type inversion) [4, 5]. But some defects may also have beneficial applications such as the observed defect-induced-photoluminescence in Si [6], which can transform Si into a light-emitter material.

The understanding of properties and dynamics of defects is a key factor for defining strategies to minimize the negative effects associated to them, and enhance the positive ones. Due to the large variety of defects that can coexist in a material, experimental structural and spectroscopic characterization techniques find it difficult to assign a given signal to a specific defect. We use multi-scale scheme to simulate and model the defect generation mechanisms due to irradiation and the defect evolution upon annealing, as well as to gain insight into the structural, energetic, electrical and optical properties of defects and thus assist experimentalists to interpret their results and provide engineers with clues for process optimization.

Within this multi-scale simulation scheme we have developed an atomistic model for the formation of extended {113} defects in silicon [7], which served to validate a novel structural characterization technique known as unprocessed high-angle annular darkfield scanning TEM [8] as shown in Fig. 1.

We have used classical molecular dynamics techniques to study the imperfect regrowth of FinFET devices [9]. TEM images show the generation of line defects in the FinFET body and the formation of polycrystalline material, which degrade its performance (left side of Fig. 2). Our simulations allowed to relate the formation of such line defects during regrowth of the FinFET body with the particular orientation of the growing amorphous-crystal interface (right side of Fig. 2), and even to give technological clues about how to improve regrowth.

We have used ab initio simulations to study the relevant defects states in amorphous Si (a-Si) and at its interface with crystalline Si, and how these defects interact with charge carriers. We have identified intrinsic hole traps in a-Si associated to locally strained regions (Fig 3), and we have analyzed their interaction with boron atoms. We have found that the low doping efficiency in the case of B is an intrinsic property of amorphous silicon since, even if it is well relaxed, locally strained regions exist [10]. This fact limits the application of amorphous silicon in devices that require higher carrier densities.

References

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Figures

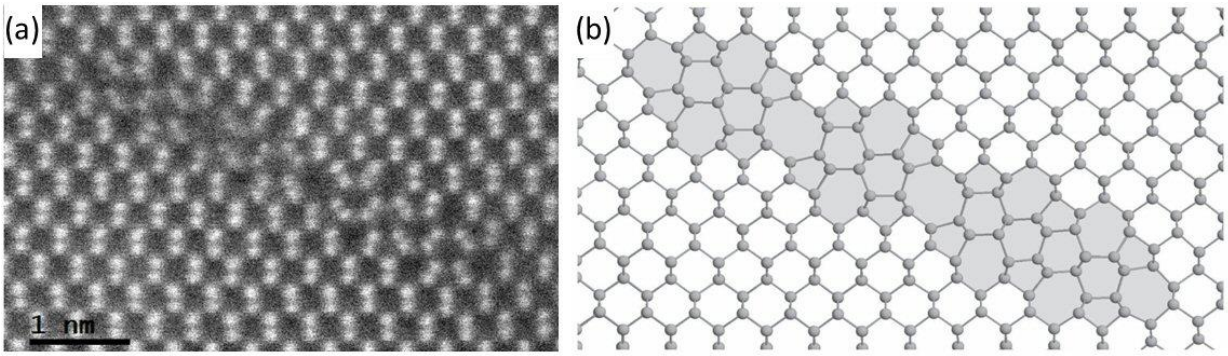

Figure 1 - (a) TEM image is compared with (b) the structural model obtained in the simulation to characterize a planar {113} defect [8].

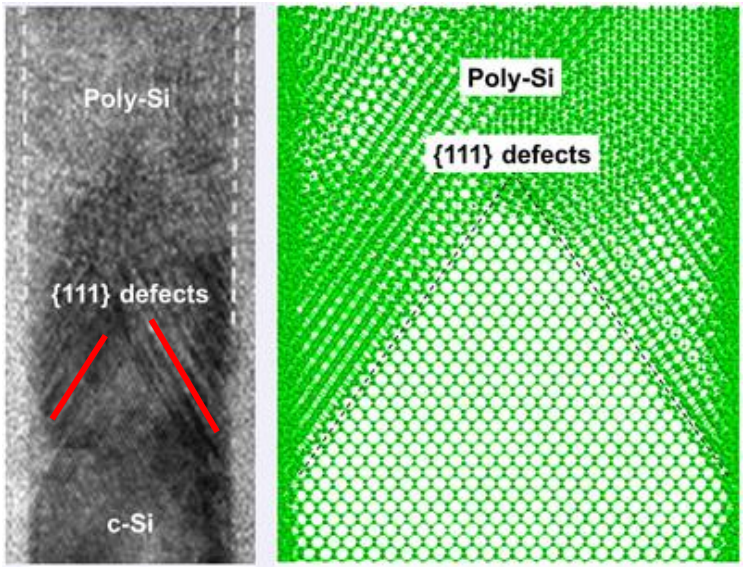

Figure 2 - (left) TEM image of a FinFET after regrowth (from R. Duffy et al., Appl. Phys. Lett. 190 (2007) 241912), and (right) classical molecular dynamics simulation results showing the line defects observed in the experiments [9].

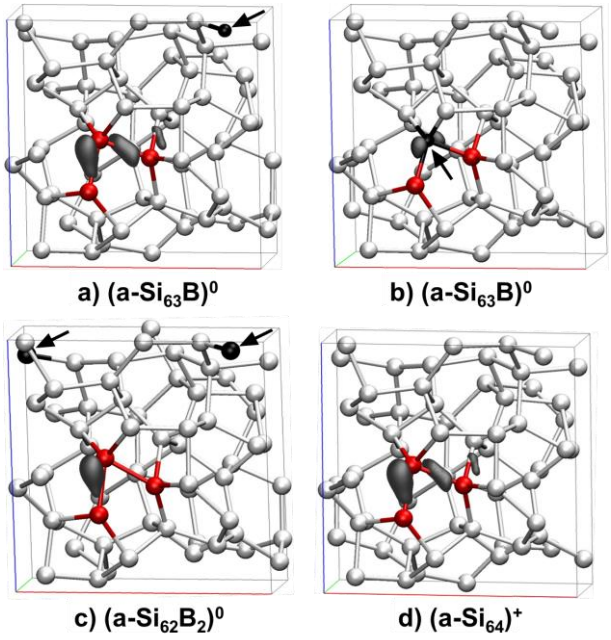

Figure 3 – Hole spatial localization in B-doped (a, b, c) and undoped (d) 64-atom cells of amorphous Si with different charge states. The dark shadowed areas show the isosurface at 50% of the maximum hole density. B atoms are black and marked by arrows, while Si atoms are white and red. It can be seen that the hole spatial localization in a-Si:B (and therefore the doping efficiency) is highly influenced by the presence locally strained regions (represented by red Si atoms). These strained regions induce around them the spatial localization of holes, independently of the position and concentration of B atoms (a, b, c), and are inherent to the a-Si matrix (d).